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MULTISCALE RESOLUTION CONTINUUM THEORY FOR ELASTIC PLASTIC MATERIAL WITH DAMAGE, AN IMPLICIT 3D IMPLEMENTATION

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Abstract: The multiscale resolution continuum theory (MRCT) [1] is a higher order continuum theory in which additional kinematic variables are added to account for the size effect at several distinct length scales. This remedies the deficiency of the conventional continuum approach when predicting both strain softening and strain hardening materials and resolves the microstructure details without extremely fine mesh in the localization zone, however additional nodal degrees of freedom are needed and the requirement of element size at the length scale somewhat adds to the computational burden. This paper is an extension of the simplified 1D multiscale implementation presented in Complas XI 2011 [14]. A 3D elastic-plastic multiscale element, with one additional subscale in which the damage is applied, is implemented implicitly in the general purpose finite element analysis program FEAP.

1 INTRODUCTION

The macroscopic properties of materials are determined by the evolving microstructures. When using the conventional continuum mechanics method, the material is assumed to be homogeneous over the volume represented by an integration point of an element. The resolution of the heterogeneous material properties requires a very fine mesh and then the computational economy is lost. The multiscale resolution continuum theory (MRCT) developed in [1], inspired by the early studies of [2] and [3], is a higher order continuum theory in which additional kinematic variables are added to account for the size effect. The MRCT introduces multiple length scales useful for applications for localization problems. It has additional nodal parameters for the information about the deformation on the microstructural scale. This reduces the problem of having an extremely fine mesh in the structure although small elements at the size of the length scale are required in order to have a convergent solution. This together with the additional nodal variables adds to the computational burden. It should be noted that classical numerical formulations without a length scale would never achieve a convergent solution for localization problems.
All the symbols and notations employed in this paper is the same as the ones used in paper presented in Complas XI 2011 [14]. The current work has implemented the theory in a numerical context where its applicability to necking/fracturing processes

will be studied and the accuracy and efficiency compared with the use of non-local damage models.

2 MULTISCALE RESOLUTION CONTINUUM THEORY

The basic idea of a higher order continuum theory is that a point in the continuum is considered as a deformable particle and a continuum is a collection of such deformable point particles. They are infinitesimal in size but assumed to have an inner structure, which can be a sequence of nested subdomains for the material point **x**. The multiscale resolution continuum theory is developed in terms of the virtual power in such a continuum during deformation [1,15,16].

2.1 Multiscale governing equations.

The linear approximation of the variation of the velocity field around the material point **x** is written as the Taylor's series about the center **x** of the microdomain and truncated at the first order to give:

$$ {}_{m}\mathbf{l}^{i}\left(\mathbf{x}+\mathbf{y}\right)=\mathbf{l}^{i}\left(\mathbf{x}\right)+\mathbf{g}^{i}\left(\mathbf{x}\right)\cdot\mathbf{y}^{i}, \tag{1}$$

where, ${}_{m}\mathbf{l}^{i}$ is the local velocity gradient for each microdomain *i*. **x** is the nested domain center and $\mathbf{y}^{i}$ is a local coordinates in the *i*th microdomain that is relative to the domain center. The term $\mathbf{l}^{i}$ is the volume average of the local velocity gradient and $\mathbf{g}^{i}$ is the gradient of velocity gradient.

The virtual internal power is now decomposed into two parts to account for both homogeneous and inhomogeneous deformations.

$$ \delta p=\delta p_{\mathrm{int}}^{\mathrm{hom}}+\delta p_{\mathrm{int}}^{inh}\,. \tag{2}$$

The homogeneous term is the conventional homogenized virtual internal power, the inhomogeneous term is defined as the difference between the volume average of the local inhomogeneous virtual internal power and the virtual internal power at the macroscopic scale:

$$ \delta p_{\mathrm{int}}^{\mathrm{hom}}+\delta p_{\mathrm{int}}^{inh}=\sigma^{0}:\delta\mathbf{l}^{0}+\sum_{i=1}^{N}\frac{1}{\Omega^{i}}\int_{\Omega^{i}}\left({}_{m}\sigma^{i}:\delta_{m}\mathbf{l}^{i}-\sigma^{0}:\delta\mathbf{l}^{0}\right)d\Omega, \tag{3}$$

where $\mathbf{l}^{0}$ is the spatial velocity gradient and σ^{0} is the Cauchy stress tensor on the macroscopic scale. The corresponding quantities, ${}_{m}\mathbf{l}^{i}$ and ${}_{m}\sigma^{i}$, are local velocity gradient and local stress for each microdomain *i*. The inhomogeneous virtual internal power $\delta p_{\mathrm{int}}^{inh}$ is rewritten in terms of the local inhomogeneous velocity gradient $\delta_{m}\mathbf{l}^{i}-\delta\mathbf{l}^{0}$ to give:

$$ \delta p_{\mathrm{int}}^{inh}=\sum_{i=1}^{N}\frac{1}{\Omega^{i}}\int_{\Omega^{i}}\left({}_{m}\beta^{i}:\left(\delta_{m}\mathbf{l}^{i}-\delta\mathbf{l}^{0}\right)\right)d\Omega, \tag{4}$$

where a microstress measure ${}_{m}\beta^{i}$ is introduced [17] as the power conjugate of the local inhomogeneous velocity gradient $\delta_{m}\mathbf{l}^{i}-\delta\mathbf{l}^{0}$. This microstress ${}_{m}\beta^{i}$ is the basis of the multiscale resolution continuum theory and can be interpreted as a measure of the resistance to the inhomogeneous deformation within the microdomain. Substitute the local velocity gradient expression Eq.(1) into Eq. (4), the inhomogeneous virtual internal power is rewritten again as:

$$\delta p_{\mathrm{int}}^{inh} = \sum_{i=1}^{N} \beta^i : \left(\delta \mathbf{l}^i - \delta \mathbf{l}^0\right) + \mathbf{m}^i \,\vdots\, \delta \mathbf{g}^i, \tag{5}$$

where the volume average microstress β^i is

$$\beta^i = \frac{1}{\Omega^i} \int_{\Omega^i} \beta_m^i d\Omega, \tag{6}$$

the microstress couple $\mathbf{m}^i$ is as the power conjugate to the gradient of the velocity gradient:

$$\mathbf{m}^i = \frac{1}{\Omega^i} \int_{\Omega^i} \beta_m^i \otimes \mathbf{y} d\Omega \tag{7}$$

and now the total virtual internal power integrated over the entire body is written as:

$$\delta p_{\mathrm{int}} = \delta p_{\mathrm{int}}^{\mathrm{hom}} + \delta p_{\mathrm{int}}^{inh} = \int_{\Omega} \left(\sigma^0 : \delta \mathbf{l}^0 + \sum_{i=1}^{N} \beta^i : \left(\delta \mathbf{l}^i - \delta \mathbf{l}^0\right) + \mathbf{m}^i \,\vdots\, \delta \mathbf{g}^i \right) d\Omega. \tag{8}$$

Integrate by parts and apply the divergence theorem to the above equation and set the virtual power to zero with the expression of virtual external and kinematic power derived in [17], resulting in the multiscale resolution continuum equilibrium equation as:

$$\begin{aligned} &\nabla \cdot \left(\sigma^0 - \sum_{i=1}^{N} \beta^i \right) + b = \rho \dot{\mathbf{v}}^0, \\ &\nabla \cdot \mathbf{m}^i - \beta^i + B^n = \gamma^i I^i \qquad i = 1..N, \end{aligned} \tag{9}$$

where $\mathbf{v}^0$ is the macroscopic velocity field, r is the macroscopic density, r^i is the density in microdomain i, b is the macroscopic body force and B^n the force couple, γ^i is the micro-acceleration defined as

$$\gamma^i = \dot{\mathbf{l}}^i + \mathbf{l}^i \cdot \mathbf{l}^i, \tag{10}$$

and the inertia tensor is

$$I^i = \frac{1}{\Omega^i} \int_{\Omega^1} \rho^i \mathbf{y}^i \otimes \mathbf{y}^i d\Omega. \tag{11}$$

2.2 Multiscale constitutions in elastic regime.

The generalized stress vector Σ is used in place of the traditional Cauchy stress σ:

$$\Sigma^T = \begin{bmatrix} \sigma^0 & \beta^i & \mathbf{m}^i \end{bmatrix}, \tag{12}$$

the different velocity gradient measures is also put into a vector form as:

$$\Delta^T = \begin{bmatrix} d^0 & d^i - d^0 & g^i \end{bmatrix}, \tag{13}$$

notice that the symmetric part of velocity gradient is used.

In elastic regime, the objective rate of the generalized stress vector and strain vector is related to the generalized velocity gradient by the elastic modulus **C**:

$$\Sigma^{\nabla} = C \cdot \Delta, \tag{14}$$

where $[\ ]^{\nabla}$ denotes any objective rate and

$$C = \begin{bmatrix} C_\sigma & 0 & 0 \\ 0 & C_\beta^i & C_{\beta m}^i \\ 0 & C_{\beta m}^i & C_m^i \end{bmatrix}, \tag{15}$$

C_σ is the conventional elasticity tensor, $C^i_\beta, C^i_{\beta m}, C^i_m$ are microscale elasticity matrices, where

$$C^i_\beta = \frac{1}{\Omega^i}\int_{\Omega^i} C^a d\Omega = C^a$$

$$C^i_{\beta m} = \frac{1}{\Omega^i}\int_{\Omega^i} C^a \otimes y d\Omega = 0, \qquad \text{for isotropic materials,} \tag{16}$$

$$C^i_m = \frac{1}{\Omega^i}\int_{\Omega^i} C^a \otimes y \otimes y d\Omega = C^a \otimes \frac{l^{i2}}{12} I$$

C^a is the average elasticity tensor in the microdomain. The determination of C^a is still phenomenological [1], in our implementation $C^a = \frac{1}{10}C_\sigma$ is used, l^i is the length scale parameter.

3 3D ELASTIC-PLASTIC MULTISCALE ELEMENT WITH DAMAGE APPLIED AT SUBSCALE

The multiscale resolution continuum is implemented in the general purpose finite element analysis program FEAP [19]. The material is considered to have one subscale in addition to the macroscopic scale. We use the hypoelastic-plactic approach. The J2 flow theory plasticity with a nonlinear hardening law [18] is used to describe the macroscopic properties. A simplified behavior of the subscale is used currently. It is assumed to be elastic with damage in the same way as in [14].

The damage is assumed to be symmetric in all 3 directions in microdomain, the fraction of damage volume is

$$\omega = \prod_{i=1}^{R}\left(1 - \frac{2y_i}{l^1}\right), \tag{17}$$

The parameter y_i is the distance from origin to where the damage has reached into the microdomain and is assumed to be equal in all 3 directions. Figure 1 below is a 2D review of the damage in the microdomain.

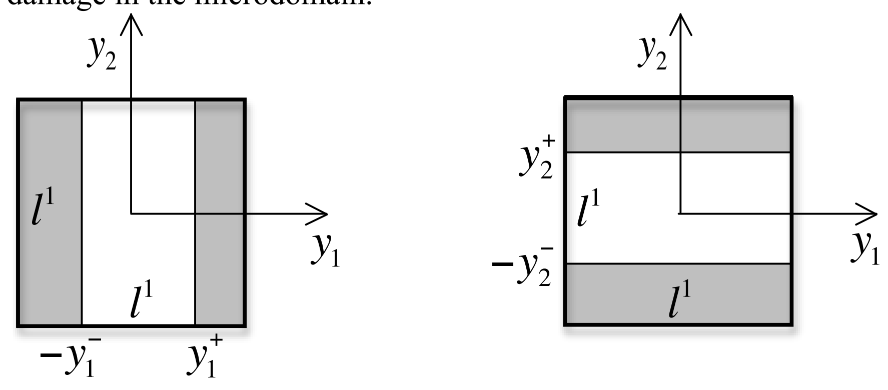

Figure 1: Two-dimensional view of damage volumes (gray) that are growing into the microdomain.

The elastic matrix for microstress becomes:

$$\mathbf{C}^1_\beta = C^a \prod_{i=1}^{R}\left(1 - \omega_i\right) = \mathbf{C}^a Z_1 Z_2 Z_3. \tag{18}$$

and elastic matrix for stress couple becomes:

$$\mathbf{C}_m^1 = \mathbf{C}^a \otimes \frac{\left(l^1\right)^2}{12}\mathbf{D} \tag{19}$$

where

$$Z_i = \frac{2y_i}{l_1} = 1 - \omega_i \tag{20}$$

and

$$\mathbf{D} = \begin{bmatrix} (Z_1)^3 Z_2 Z_3 & 0 & 0 \\ 0 & Z_1 (Z_2)^3 Z_3 & 0 \\ 0 & 0 & Z_1 Z_2 (Z_3)^3 \end{bmatrix} \tag{21}$$

4 IMPLEMENTATION IN FEAP

The present 3D multiscale elastic-plastic formulation has one subscale. A vector $\mathbf{v}_e$ is the element interpolation of nodal values $\boldsymbol{v}$ as

$$\mathbf{v}_e = \sum_{i=1}^{n} \mathbf{N}_i \mathbf{v}_i \tag{22a}$$

where the vector of nodal variables is

$$\mathbf{v}_i = \begin{bmatrix} v_x^0 & v_y^0 & v_z^0 & d_{xx}^1 & d_{yy}^1 & d_{zz}^1 & d_{xy}^1 & d_{yz}^1 & d_{xz}^1 \end{bmatrix}^T \tag{22a}$$

where $\mathbf{v}^0$ is the macroscopic velocity at the nodes and d^1 is the subscale degrees of freedom that describe the rate of microstrains.

The symmetric part of macroscopic spatial velocity gradient is calculated in a regular way as:

$$d_e^0 = \sum_{i=1}^{n} \begin{bmatrix} \frac{\partial N_i}{\partial x} & 0 & 0 \\ 0 & \frac{\partial N_i}{\partial y} & 0 \\ 0 & 0 & \frac{\partial N_i}{\partial z} \\ \frac{\partial N_i}{\partial y} & \frac{\partial N_i}{\partial x} & 0 \\ 0 & \frac{\partial N_i}{\partial z} & \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} & 0 & \frac{\partial N_i}{\partial x} \end{bmatrix} \begin{bmatrix} v_x^0 \\ v_y^0 \\ v_z^0 \end{bmatrix} = B^0 \mathbf{v}^0 . \tag{23}$$

Gradient of microstrain $\mathbf{g}^1$ is not an independent variable but calculated from interpolation over element. The needed microstrain and strain gradient is written as:

$$\begin{aligned} d_e^1 &= \sum_{i=1}^{n} N_i^1 d^1 \\ g_e^1 &= \sum_{i=1}^{n} G_i^1 d^1 . \end{aligned} \tag{24}$$

The extended strain rate vector is written as:

$$\Delta = \begin{bmatrix} d^0 \\ d^1 - d^0 \\ g^1 \end{bmatrix} = \begin{bmatrix} B^0 & \\ -B^0 & N^1 \\ & G^1 \end{bmatrix} \begin{bmatrix} v^0 \\ d^1 \end{bmatrix} = \mathbf{Q}v, \tag{25}$$

The current problem is assumed to be quasi-static, so only internal force is calculated as:

$$\mathbf{f}_{\text{int}} = \int_\Omega \mathbf{Q}^T \Sigma \, d\Omega = \int_\Omega \begin{bmatrix} \left(B^0\right)^T \left(\sigma^0 - \beta^1\right) \\ \left(N^1\right)^T \beta^1 + \left(G^1\right)^T m^1 \end{bmatrix} d\Omega \tag{26}$$

and the element tangent stiffness matrix is calculated as:

$$K = \int_\Omega \mathbf{Q}^T C \mathbf{Q} d\Omega =$$

$$\int_\Omega \begin{bmatrix} \left(B^0\right)^T C_\sigma^{al} B^0 + \left(B^0\right)^T C_\beta^{al1} B^0 & -\left(B^0\right)^T C_\beta^{al} B^0 \\ -\left(N^1\right)^T C_\beta^{al} B^0 & \left(N^1\right)^T C_\beta^{al} N^1 + \left(G^1\right)^T C_m^{al} G^1 \end{bmatrix} d\Omega, \tag{27}$$

where $C_\sigma^{al}, C_\beta^{al1}, C_m^{al1}$ is the algorithmic modulus calculated at each scale.

5 RESULTS

A 3D bar with length 53.334, height 6.413 and width 2 is being pulled at two ends, only 1/8th of the geometry is modeled due to symmetry and the mesh is shown in Figure 2. The geometry is taken from [18]. A geometric imperfection of 1.8% reduction of height is introduced at the center of the bar to trigger the localization and a displacement of 7 is imposed at the right side of the bar. A simple damage model is used and applied at the subscale. It is

$$\omega = \left\langle \frac{\varepsilon^0 - \varepsilon_{init}}{\varepsilon_{fracture} - \varepsilon_{init}} \right\rangle \tag{28}$$

The symbol $\langle \ \rangle$ denotes that the expression is zero for negative arguments. The damage is only applied in the center region of the rod. ε^0 is the effective macroscopic strain, ε_{init} is the damage initialization strain and $\varepsilon_{fracture}$ is the strain at the fracture.

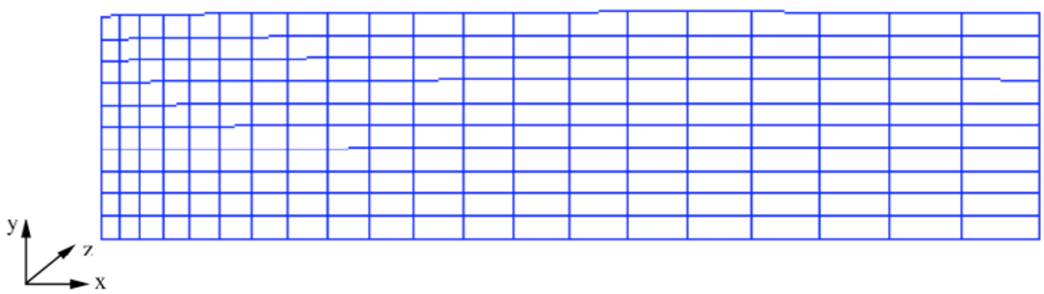

Figure 2: Mesh of the bar.

The axial stress variation along the centre axis of the bar is plotted in Figure 3. *feap2* denotes the solution given by FEAP's own large deformation element and the results from *user2* is given by our implemented hypoelastic-plastic formulation routine with only the macroscopic part of the multiscale element. This is used to verify coding of this part of the element routine. *length2*, *length4* and *length6* represent the results give by multiscale elements with the length scale in Eq. (16) set to 2, 4 and 6 respectively. Figure 4 shows stress in the axial direction with the length scale parameter of 2. The used length scales 6, 4 respectively 2 are all larger than the element sizes in the necking region.

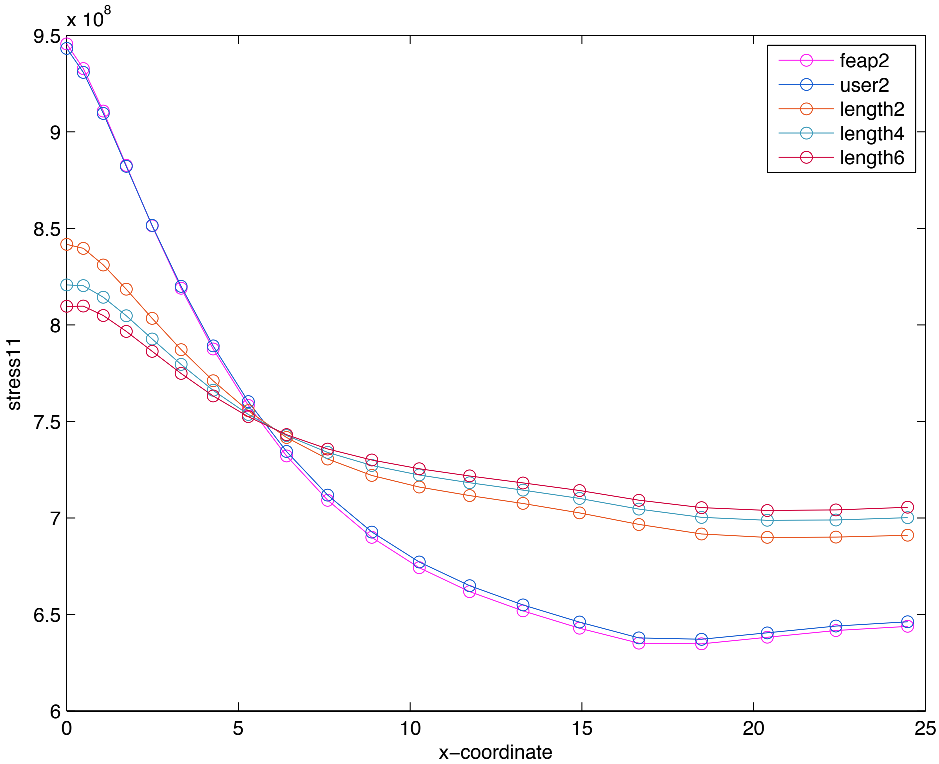

Figure 3: Stress curve along the centre axis of the bar.

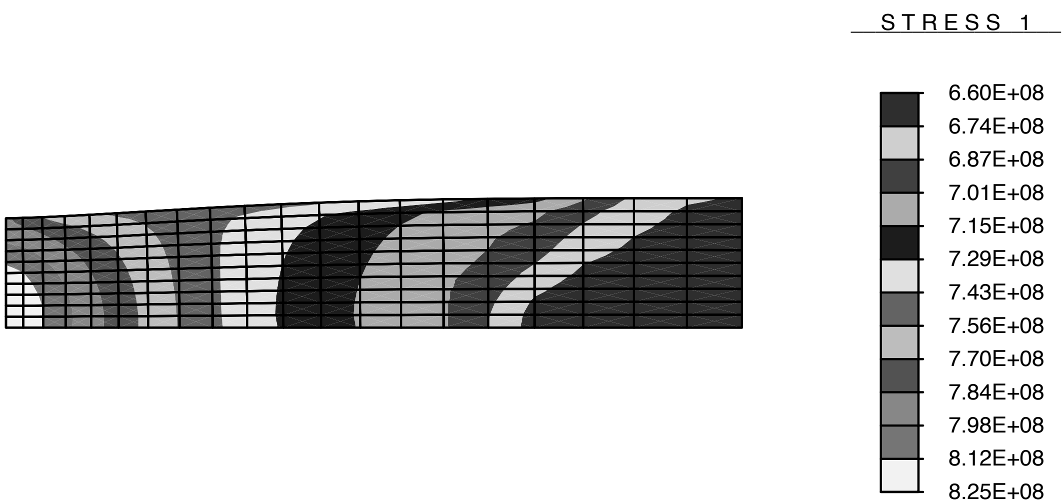

Figure 4: Axial stress with length scale of 2.

Damage from the subscale, according to Eq. (28), along the centre axis is plotted in Figure 5. The damage is highest in the center region and is zero further away from the localization. This causes the macroscopic stresses to be reduced in this region compared to the *feap2* and *user2* cases in Figure 3. Without damage the subscale is elastic and this explains the macroscopic stress further away the center region becomes higher.

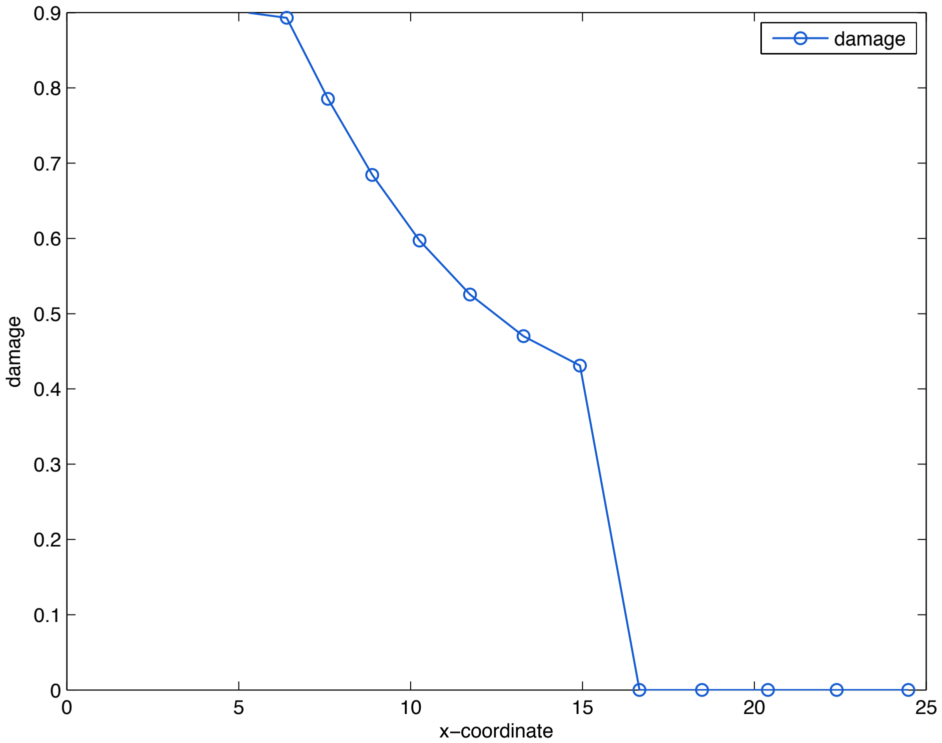

Figure 5: Damage along the center axis for length scale of 2.

6 DISCUSSIONS

A three-dimensional implementation of a multiscale element has been implemented into FEAP and initial verification tests have been done. The plastic hardening behavior is in the macroscopic part of the model whereas the damage is traced in the subscale domain. This gives a length scale useful for stabilization the numerical solution when the deformation is localized. The formulation will be applied to tensile tests on steels where the necking has measured by optical methods tracking the deformation and the strain field during the necking. The accuracy of the model, eventually with improved material models compared to the current study, and its efficiency will be evaluated. Comparative studies with non-local damage models within the classical continuum theory will also be done.

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